Tsallis distribution and luminescence decays

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Abstract

Usually, the Kohlrausch (stretched exponential) function is employed to fit the luminescence decays. In this work we propose to use the Tsallis distribution as an alternative to describe them. We show that the curves of the luminescence decay obtained from the Tsallis distribution are close to those ones obtained from the stretched exponential. Further, we show that our result can fit well the data of porous silicon at low temperature and simulation result of the trapping controlled luminescence model.

Key words: Luminescence decay, Tsallis distribution, stretched exponential

1 Introduction

The Kohlrausch (stretched exponential) function has been largely employed to describe luminescence decays of different materials and in different time scales (see [1,2,3,4,5,6,7], and references therein), and it has the following form:

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$$I_\beta(t) = I_{\beta 0} \exp\left[-\left(\frac{t}{\tau}\right)^\beta\right] \ , \tag{1}$$

with $0 < \beta < 1$. We note that the value of parameter β in the range $0 < \beta < 1$ makes $I(t)$ decays slower than the exponential function, whereas for $\beta > 1$ the function (1) is called compressed exponential and it has short-tails, consequently, it decays faster than the exponential function.

For the general consideration of the study of luminescence decay $I(t)$, it is usually considered the distribution of rate constants $H(k)$ [4] connected with $I(t)$ by the Laplace transform given by

$$I(t) = \int_0^\infty H(k) \mathrm{e}^{-kt} \mathrm{d}k \ , \tag{2}$$

with $I(0) = 1$. In particular, $H(k)$ must be nonnegative for all $k > 0$ in order to be considered as a distribution function. Moreover, the function $H(k)$ is normalized, i.e., $\int_0^\infty H(k)\mathrm{d}k = 1$. We note that $H(k)$ may have a large change for a small change in $I(t)$. In this way, the precision of the experimental data will be important for the choice of the distribution of rate constants $H(k)$.

Modification and generalization of the stretched exponential function as a decay function has been recently considered, for instance, a decay function unifying the modified stretched exponential and Becquerel decay laws [4,5,6].

In this work we consider a simple distribution of rate constants $H(k)$ based on the Tsallis distribution [8,9]. Our idea of employing this distribution is due to its simplicity and it has been applied to a variety of natural systems (see, for instance, [10,11,12,13]). We shall show that the luminescence decay function generated by the Tsallis distribution can be useful to describe experimental data. To do so we shall fit the data of porous silicon at low temperature [3] and

the simulation result of the trapping controlled luminescence model described in [1] with our luminescence decay function.

2 Distribution of rate constants $H(k)$ given by the Tsallis distribution

For the luminescence decay $I(t)$ given by Eq. (1) the distribution $H(k)$ can be expressed in an integral representation [4] as follows:

$$H_\beta(k) = \frac{\tau_0}{\pi}\int_0^\infty du \exp\left[-u^\beta \cos\left(\frac{\beta\pi}{2}\right)\right]\cos\left[u^\beta \sin\left(\frac{\beta\pi}{2}\right) - k\tau_0 u\right] . \quad (3)$$

We see that this last expression is quite complicated. Now we consider the Tsallis distribution for $H(k)$, and it is given by

$$H_q(k) = B\left[1-(1-q)\alpha k\right]^{\frac{1}{1-q}} \quad (4)$$

where $\alpha > 0$ and $0 < q < 2$, and B is a normalization factor. The parameter α has the dimension of time. For $q \longrightarrow 1$ we recover from Eq. (4) the exponential function which is connected with a particular case of the Becquerel decay function [6] given by

$$I(t) = \frac{1}{\left(1+\frac{\gamma t}{\alpha}\right)^{\frac{1}{\gamma}}} . \quad (5)$$

We note that $H_q(k)$ has a cutoff for $q < 1$, i.e., the term $[1-(1-q)\alpha k]^{\frac{1}{1-q}}$ is replaced by zero when $[1-(1-q)\alpha k] < 0$, then the normalization factor is

equal to

$$B = \alpha(2-q) \tag{6}$$

where $0 < q < 2$. The luminescence decay $I(t)$ is obtained by substituting Eq. (4) into Eq. (2), and we arrive at

$$I_q(t) = \frac{2-q}{1-q} e^{-\frac{t}{\alpha(1-q)}} \int_0^1 du\ u^{\frac{1}{1-q}} e^{\frac{tu}{\alpha(1-q)}}\ ,\ \ 0 < q < 1, \tag{7}$$

and

$$I_q(t) = \frac{2-q}{q-1} e^{-\frac{t}{\alpha(q-1)}} \int_1^\infty du\ u^{\frac{1}{1-q}} e^{\frac{tu}{\alpha(1-q)}}\ ,\ \ 1 < q < 2. \tag{8}$$

In order to see the behavior of $I_q(t)$ we plot some curves of $I_q(t)$ and $I_\beta(t)$ with typical values of α, q and β which are shown in Fig. 1. All the curves decay monotonically with time, and two of the curves of $I_q(t)$ have fat tails. We note that the lowest curve of $I_q(t)$ in the figure is very close to the curve of $I_\beta(t)$; This means that any experimental data fitted with these curves must have a good level of precision in order to choose which one of the curves is preferable.

For application of our result we consider the experimental data of porous silicon at low temperature given in [3]. In Fig. 2 we compare the best fit of the data by using the stretched exponential and $I_q(t)$. We see that both curves can fit the data (which are not shown in our figure) very well. Then, in this case, the experimental data do not offer us sufficient precision to discard one of the curves. We note that the behavior of $I_q(t)$ is not the same of $I_\beta(t)$, i.e., $I_\beta(t)$ describes a straight line, whereas $I_q(t)$ does not.

Another application of our result is to consider the model of trapping controlled luminescence given in Ref. [1]. The process during the excitation is described by the following equations:

$$\frac{\mathrm{d}n_\nu}{\mathrm{d}t} = x - R\,(M-m)\,n_\nu \tag{9}$$

$$\frac{\mathrm{d}m}{\mathrm{d}t} = -A_m m n_c + R\,(M-m)\,n_\nu \tag{10}$$

$$\frac{\mathrm{d}n}{\mathrm{d}t} = A_n\,(N-n)\,n_c \tag{11}$$

$$\frac{\mathrm{d}n_c}{\mathrm{d}t} = \frac{\mathrm{d}m}{\mathrm{d}t} + \frac{\mathrm{d}n_\nu}{\mathrm{d}t} - \frac{\mathrm{d}n}{\mathrm{d}t}\ , \tag{12}$$

where n_c and n_ν are the instantaneous concentrations of electrons in the conduction band and holes in the valence band, respectively; A_n is the retrapping coefficient, A_m is the recombination coefficient and R is the trapping coefficient of free holes during the excitation; N and M are the concentrations of the traps and recombination centers, whereas n and m are their respective instantaneous occupancies. Finally x is the rate of production of electrons and holes by the excitation irradiation. The luminescence emission intensity is calculated by the rate of electron-hole recombination given by

$$I = -\frac{\mathrm{d}m}{\mathrm{d}t} = -A_m m n_c\ . \tag{13}$$

In Fig. 3 shows a replotting of the simulation result [1] and the best fitted stretched exponential function with the parameters $x = 10^{19}\mathrm{m}^{-3}\mathrm{s}^{-1}$, $A_m = 10^{-17}\mathrm{m}^3\mathrm{s}^{-1}$, $A_n = 10^{-9}\mathrm{m}^3\mathrm{s}^{-1}$, $R = 10^{-17}\mathrm{m}^3\mathrm{s}^{-1}$, $N = 10^{18}\mathrm{m}^{-3}$, $M = 10^{19}\mathrm{m}^{-3}$. We note that the agreement is not very good. In order to enhance the fitting result the decay curve has been separated into two parts [1]: The values have been fitted separately for the first microsecond and for the period of time from $t = 2$ to 10μs. In Fig. 4 shows the simulation result fitted by our result; we see that the agreement is excellent and the decay curve has not been separated.

3 Conclusion

In this work we have considered the Tsallis distribution as a distribution of rate constants $H(k)$. From Eq. (2) we have obtained the luminescence decay function $I_q(t)$ for fitting the luminescence decays. We have shown that $I_q(t)$ may have fat tails and its behavior looks like the stretched exponential function. We have also demonstrated that $I_q(t)$ can be useful to describe experimental data. In the case of the trapping controlled luminescence model the fitted result by $I_q(t)$ is superior than the best fitted stretched exponential function. It can be seen that, Fig. 3, the deviation of the best fitted stretched exponential function from the exponential one is not small $\beta = 0.45$. On the other hand, Fig. 4 shows the simulation result fitted by $I_q(t)$ with $q = 1.04$ which presents a small deviation of $H_q(k)$ from the exponential function, then $H_q(k)$ is close to the Becquerel distribution of rate constants $\alpha \exp(-k\alpha)$; however, the parameter $\alpha = 13.0321\mu$s has a value close to $\tau = 11.8\mu$s.

Acknowledgment

The author acknowledges partial financial support from the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), Brazilian agency.

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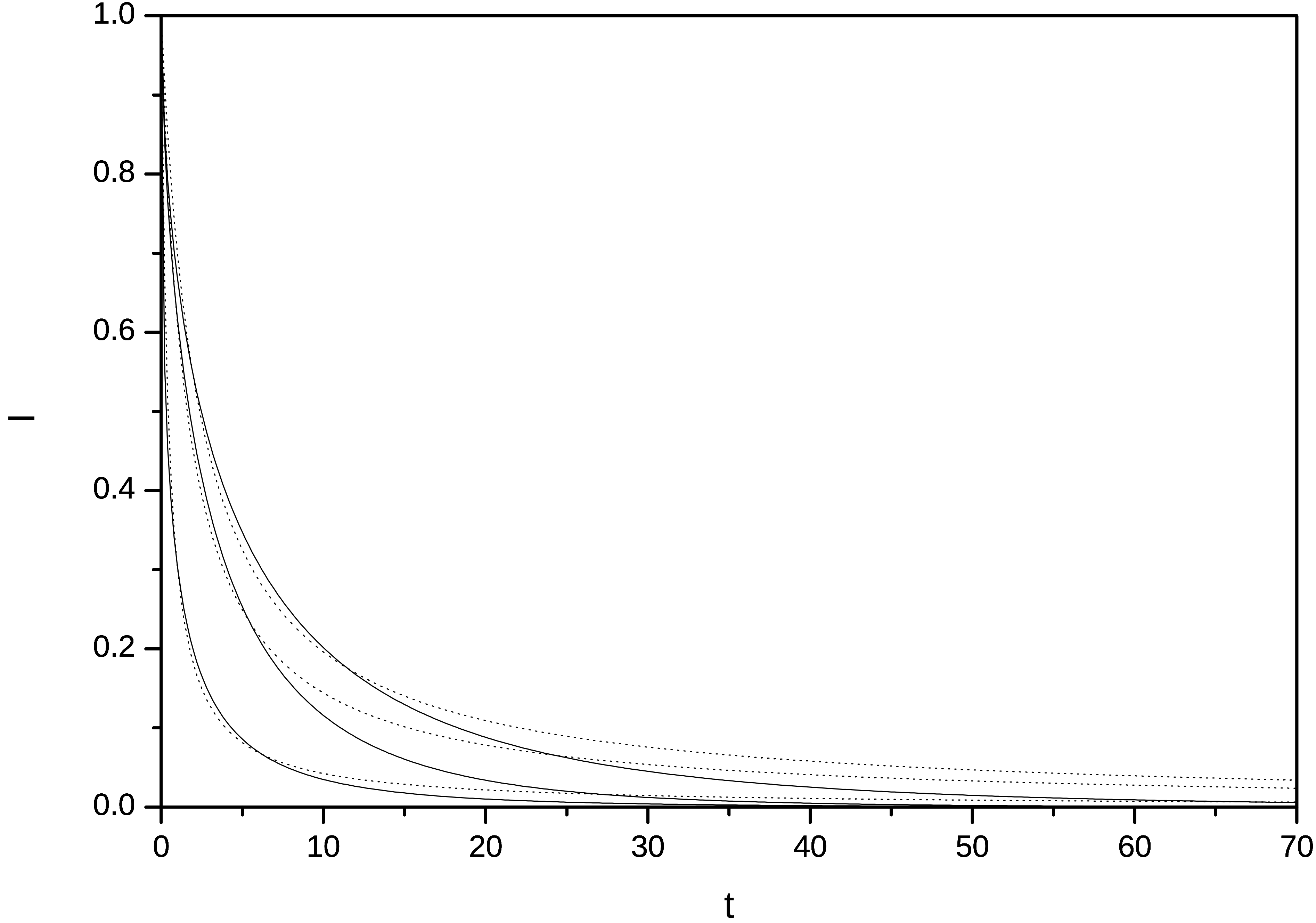
Figure Captions

Fig. 1 - Plots of $I_q(t)$ and $I_\beta(t)$ given by Eqs. (1) and (8) in arbitrary units. The dotted lines correspond to $I_q(t)$, whereas the solid lines correspond to $I_\beta(t)$ with typical parameter values: from top to bottom, $\beta = 0.6$, $\tau = 4.56$, $\alpha = (1.64)^2$, $q = 1 + (0.28)^2$; $\beta = 0.65$, $\tau = 3.07$, $\alpha = (1.4)^2$, $q = 1 + (0.35)^2$; $\beta = 0.45$, $\tau = 0.68$, $\alpha = (0.695)^2$, $q = 1 + (0.275)^2$.

Fig. 2 - The best fit to Eq. (1) (solid line) for porous silicon at low temperature described in [3] with $\beta = 0.75$ and $\tau = 2.4$ms. The dotted line is the plot of Eq. (8) with $q = 1 + (0.25)^2$ and $\alpha = (1.235)^2$ms.

Fig. 3 - Replotting of the simulation result calculated in [1] and the best fitted stretched exponential function with $\beta = 0.45$ and $\tau = 11.8$ μs.

Fig. 4 - Plots of the simulation result calculated in [1] (solid line) and $I_q(t)$ (dotted line) with $q = 1 + (0.2)^2$ and $\alpha = (3.61)^2\mu$s.



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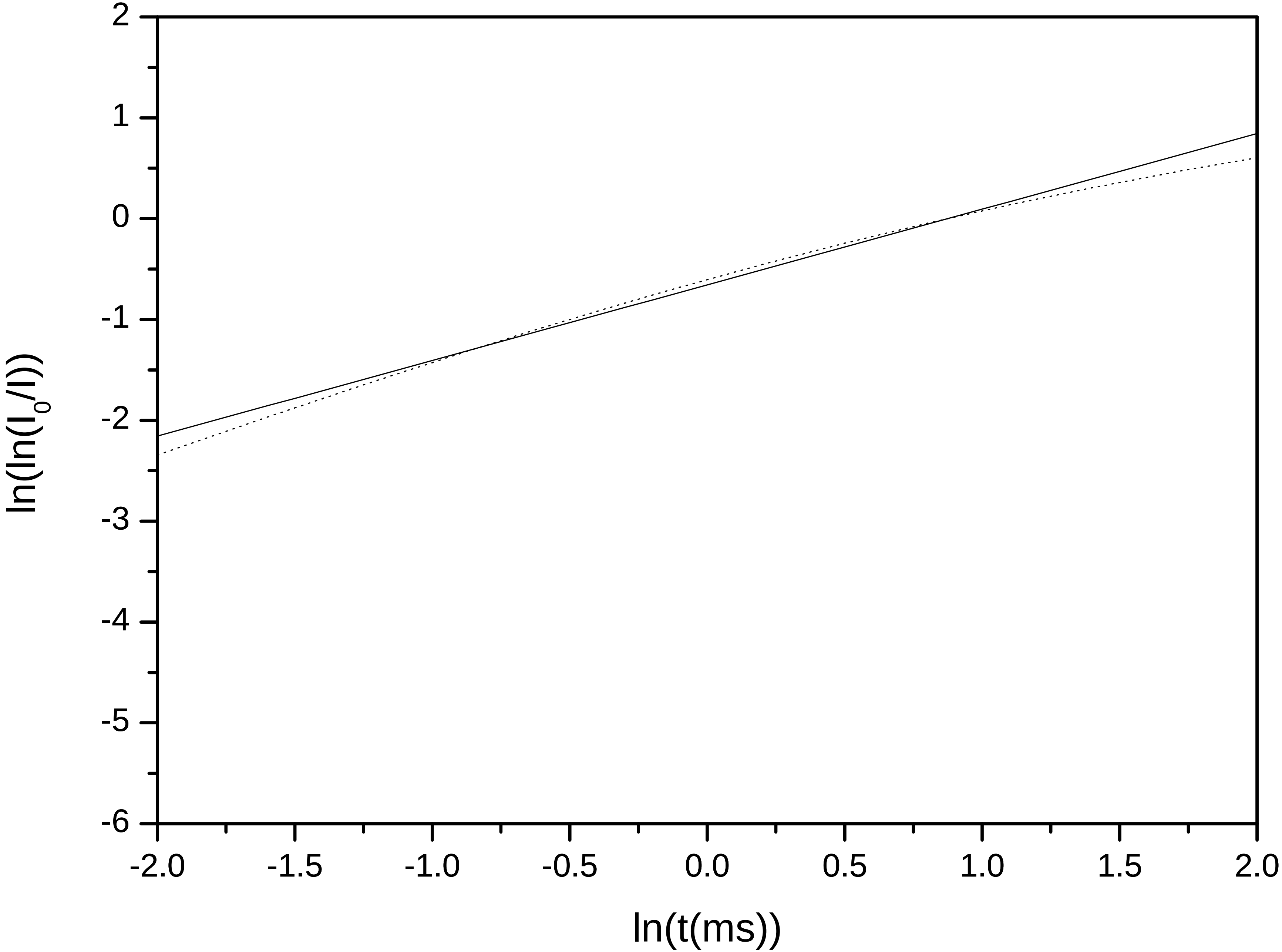
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$\ln(\ln(I_0/I))$
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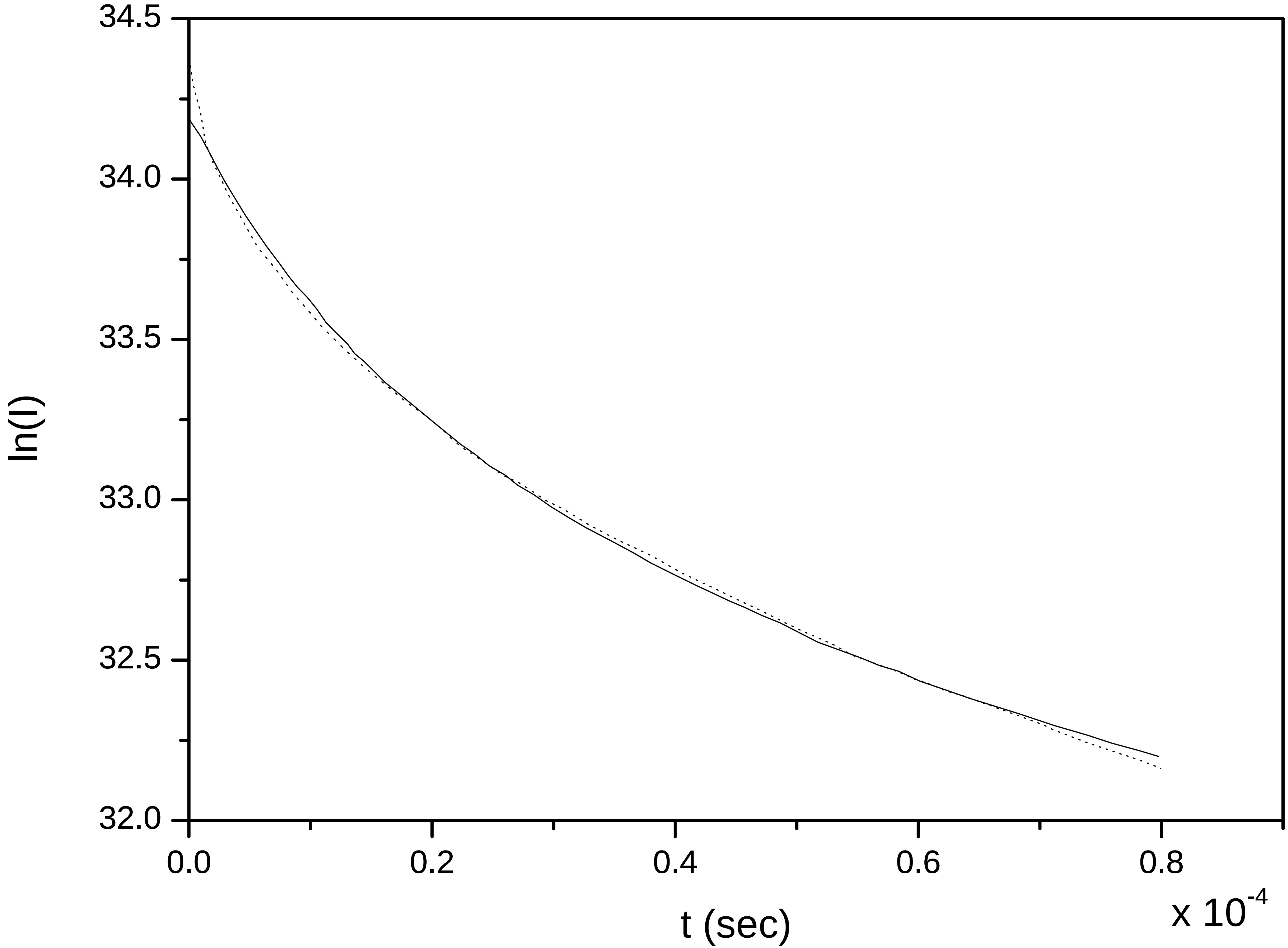

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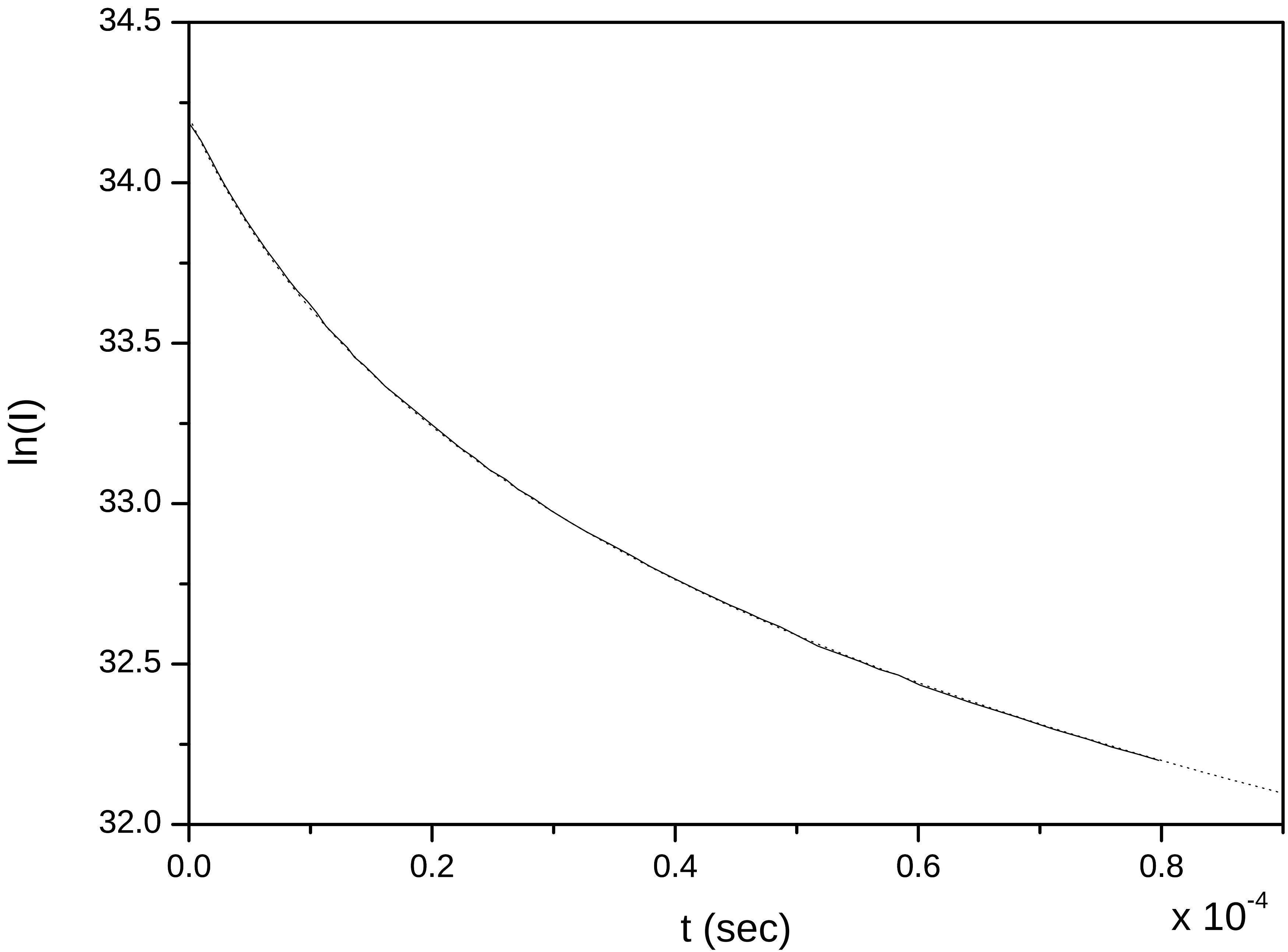

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